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BASIN-SCALE GEOTHERMAL MODEL CALIBRATION USING ITOUGH2

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ABSTRACT

We showcase how the application of parameter-estimation and sensitivity-study methods implemented in iTOUGH2 improved model calibration to measured data and provided insight into model uncertainties and data outliers. The methodology was applied to a basin-scale conductive heat model of temperature in the Perth Basin, Western Australia.

MOTIVATION AND INTRODUCTION

Geothermal resource estimations require a trade-off between conceptualizing the complicated geological system with a finite numerical representation, and estimating these model parameters from scarce data. There is often a high degree of uncertainty about the heat flow parameters used in the simulation, especially for large-scale systems with poorly detailed boundary conditions (see, e.g., Kohl, 2003).

A suitable input parameter set may be estimated by first performing a forward simulation of temperatures, and second by comparing simulated to measured values in wells. A common approach is to simply compare values by “eyeballing”, for example by plotting simulated next to measured values along a temperature log (Saibi, 2011), or by comparing a sum of simulated mismatch across all data points (Reid et al., 2012a). The input parameters are then adjusted by trial-and-error until a reasonable fit is obtained. Although this method seems to be very “ad-hoc,” it is usually possible to obtain acceptable results with a reasonable amount of manual calibration steps. For purely conductive geothermal models, this approach may be adequate, as the forward simulation is approximately linear in its response to the parameters and the sensitivities of the single model parameters can be reasonably well determined.

This simple manual calibration method can be automated with several more sophisticated model calibration methods. The advantages of automatic calibration are a requirement to mathematically define what constitutes a “good” fit, systematic analysis of the sensitivity of the computational model to both the parameters and the calibration data, an indication of the adequacy of the conceptual model, and calibrated parameters which hopefully provide an adequate fit to measurements—of course all at the expense of computational complexity. We do not claim that automatic calibration methods produce a “true” or unique model (Moore and Doherty, 2005), but the approach, when applied carefully, will produce a well-considered model.

In this work we apply the iTOUGH2 program (Finsterle, 1999) to automatically calibrate a complex geothermal model using the PEST protocol (Finsterle and Zhang, 2011). The conductive forward simulations are performed in SHEMAT (Clauser and Bartels, 2003), as multiphase flow is not considered at this stage. We utilize the stand-alone capabilities of iTOUGH2 to estimate thermal rock parameters and boundary conditions. Our aim is to produce a simplified basin-scale model to act as a basis for future detailed reservoir-scale simulations representing more complex physical heat transport mechanisms, such as convection and groundwater advection.

GEOTHERMAL MODELING PROJECT

We developed three-dimensional models of the geology and the conductive temperature regime of the entire Perth Basin in Western Australia, with an extent of nearly 800 km from north to south and 150 km east to west. The enormous physical scale required many simplifications to integrate the three-dimensional geological model and discrete geothermal simulation.

The geological model is based on an amalgamation of data from petroleum exploration wells, existing geological studies, and new fault interpretations. Full details are provided in Reid et al. (2012a, 2012b). The model covers an area of over 100,000 km^2 and extends to a depth of 120 km. The stratigraphic column includes twelve sedimentary units. Because of the large latitudinal extent of the Basin and computational limitations, the model was developed in three overlapping regions representing the South, Central, and North Perth Basins.

The geological model is discretized into a deep model down to 120 km, below the Mohorovičić discontinuity, and a shallow model down to 16 km [Figure **1**]. The deep model provides the lower boundary condition of vertical heat flux to the shallow model, which has a finer resolution and contains the sedimentary geologic units. Horizontal mesh resolution is 500 × 500 m, and vertical resolution is 25 m at the surface and 1 km at the base, leading to a total of approximately 50 million cells. Mean annual surface temperature determined from remote sensing data (Horowitz, 2009) is applied as an upper boundary condition. Regional studies and local measurements provide initial estimates of thermal properties as detailed below. The steady-state conductive temperature distribution with these properties and boundary conditions was calculated using SHEMAT.

PARAMETER IDENTIFICATION

When building the geologic model, we intentionally kept the number of rock formations as small as possible while still adequately representing the thermal regime at measured depths. Because the Perth Basin has a depth of up to 16 km, the deeper formations are poorly constrained geometrically and petrophysically. However, in the central part of the Basin near the city of Perth, previous research had developed a sophisticated geologic model with considerable detail in the shallow sedimentary layers (Reid et al., 2012b). Geothermal measurements suggest that heat moves in the Perth Basin via simple conduction, but also via nonlinear physical processes such as groundwater advection and density-driven convection (Sheldon et al. 2012b). Nonetheless, our initial modeling efforts focus only on steady-state heat conduction, due to the difficulty in identifying hydrogeologic boundary conditions at the basin scale, and the lack of transient temperature measurements.

For steady-state heat conduction, only three rock properties are relevant: radiogenic heat production, thermal conductivity, and porosity. SHEMAT requires radiogenic heat production rates and thermal conductivity to be expressed as pure rock properties, which can be derived from bulk matrix values by correcting with porosity. Manually calibrated estimates of these rock properties for the 12 stratigraphic units are provided in Table **1**. The values were derived from specific studies within the Perth Basin and Australia, and in some cases from worldwide representative ranges; further discussion is provided in Reid et al. (2012a).

Additional boundary condition parameters to the model were the upward basal heat flux at 55 km in depth. Again, a parsimonious model was assumed, with basal heat flux described by a planar function that varied only in the north-south direction along the basin axis.

CALIBRATION DATA SET

Few meaningful measurements of heat transport properties were available within the range of the basin. However, more than 130 point temperature observations exist in the area. Temperature measurements in the Perth Basin are available from deep petroleum exploration wells, usually from bottomhole temperature (BHT) measurements or from drill stem tests (DST). Observations are acquired shortly after the well is drilled, due to equipment logistics and costs. The well measurements do not exhibit consistent reliability and can often underestimate temperature by 15% (Ricard et al., 2012). Several reliability classifications exist that take into account the type of measurements and reservoir conditions. We selected 135 high reliability temperature measurements from 97 wells across the whole Perth Basin. The spatial coverage of the measurements varies considerably. While 114 high-quality measurements are available in the North Perth Basin, only 5 are available in the South Perth

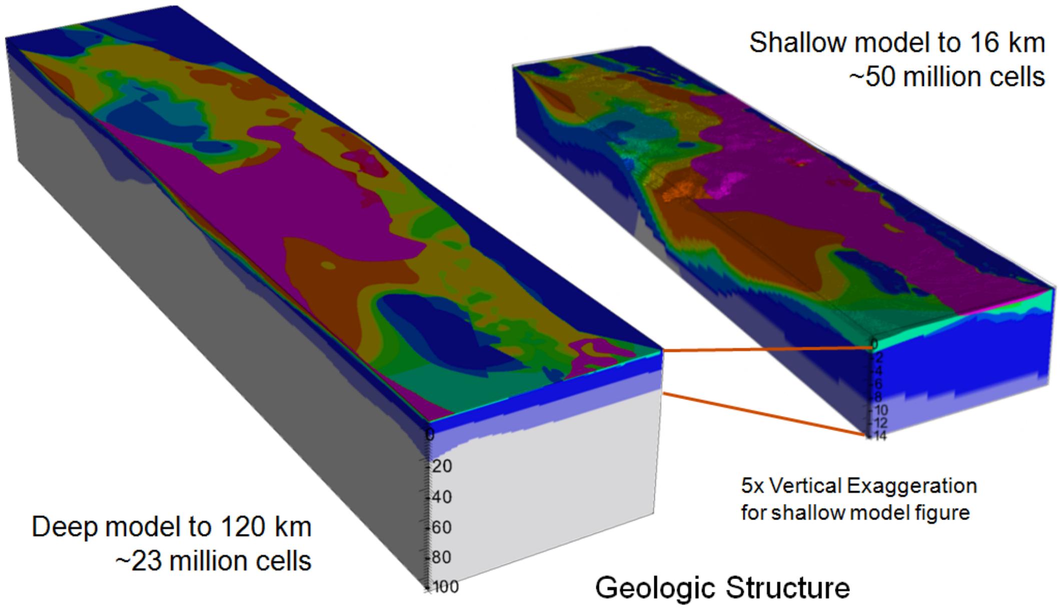

Figure 1. Deep and shallow geologic models, showing extent of formations

Table 1. Initial manual and final automatic calibrated parameter values. The upper crust radiogenic heat production was initially 2.4×10^{-6}; the final calibrated 2.2×10^{-6} $\mu W\ m^{-3}$

Formation	Porosity (-)	Radiogenic heat production ($\mu W\ m^{-3}$)	Manual Calibrated Thermal Conductivity ($W\ m^{-1}\ K^{-1}$)	Automatic Calibrated Thermal Conductivity ($W\ m^{-1}\ K^{-1}$)
Mantle	0.01	0.0	4.0	N/A
Lower Crust	0.01	1.5×10^{-7}	3.2	N/A
Upper Crust - Basement	0.01	See legend	2.7	3.0
Sue Group (Permian)	0.05	4.0×10^{-7}	3.1	2.6
Kockatea Shale	0.12	1.2×10^{-6}	1.5	1.3
Late Triassic Formations	0.05	5.0×10^{-7}	4.3	N/A
Lesueur Formation	0.09	5.0×10^{-7}	3.8	4.2
Eneabba Formation	0.06	5.0×10^{-7}	3.6	3.4
Cattamarra Coal Measures	0.10	4.5 x 10-7	4.1	2.3
Yarragadee Formation	0.20	5.0×10^{-7}	4.3	4.9
Parmelia Formation	0.20	5.0×10^{-7}	3.1	N/A
Gage Sandstone	0.10	5.0×10^{-7}	3.9	N/A
South Perth Shale	0.10	8.0 x 10-7	1.5	N/A
Leederville Formation	0.30	6.0×10^{-7}	3.4	N/A
Superficial Formation	0.30	6.0×10^{-7}	3.4	N/A

Basin and 16 in the Central Perth Basin. No temperature measurements were available outside the Perth Basin sedimentary rocks, e.g., in the eastern Yilgarn Craton. All the measurements are located at depths less than 4.8 km, with the majority at economic petroleum exploration depths between 1.5 and 3.5 km.

These measurements were corrected to provide true formation temperature estimates, which are always higher than the initial measurements. More importantly, uncertainty on the correction was also calculated, which depended upon the measurement technique, number of samples, and the depth of measurement (Richard et al., 2012). Over the 135 measurements, the average measurement error was 5°C. A full table of the measurements, the corrected true formation temperature, and the standard deviation of the measurement error is provided in Reid et al. (2012a). Our aim in the calibration was to reproduce these temperature measurements by simulation, within the limits of measurement uncertainty.

MANUAL CALIBRATION

The model was calibrated in two stages: first via manual calibration and then by the automatic technique described below. In the initial calibration procedure, thermal conductivity, radiogenic heat production rate (HPR) of the upper crust, and deep basal heat flux were altered to better match the measured temperatures. Porosity and HPR in shallower sediments were fixed at initial estimates, due to their limited effect on the model output. The simulated temperature was obtained at the measurement location through trilinear interpolation from the surrounding model node values. Subtracting the simulated from the measured temperature produced a temperature residual at each well, which is then considered in conjunction with the estimated measurement error. Simulated temperatures were considered "very good" if they fell within one standard deviation of the corrected BHT, and "good" if within two standard deviations. Two additional measures of goodness-of-fit were provided by (1) the average temperature error in the model domain and (2) a squared residual weighted by the measurement error.

The simulated temperature and residual difference from the true formation temperature from the manual calibration are shown in Reid et al. (2012a). Mean residual was -5.3°C, showing that the manual calibration systematically underestimated the temperature. The standard deviation of the residuals was 12.8°C, which also demonstrated that the manual calibration did not reproduce all measurements within a 95% measurement error confidence. Only 24% of simulated measurements were very good and lay within one standard deviation of TFT, and 45% were reproduced within two standard deviations. Initial sensitivity runs during manual calibration suggested that the most important parameters for calibration were the basal heat flux at 120 km and the radiogenic heat production value of the upper crust.

Based on the poor performance of the manual calibration, automatic calibration was begun using iTOUGH2. We used iTOUGH2 as the parameter estimation engine, controlling the SHEMAT simulations through the recently developed PEST interface (Finsterle and Zhang, 2011).

SENSITIVITY OF PARAMETERS

The first step in the calibration was a sensitivity study performed with iTOUGH2, to determine whether all parameters could be identified from the scattered measurements. We performed the study using the least-square goodness-of-fit objective function, where temperature measurements are weighted by the measurement errors derived above. Because of the relatively shallow distribution of measurements, and because conductive heat diffuses upwards, we presumed that identification of the deeper formation properties would be difficult due to auto-correlation. However, the shallow formations do not influence results in the northern and southern sub-basins due to the limited detail in those areas.

Figure **2** confirms our physical intuition: the two major sources of heat in the conductive model (basal heat flux and radiogenic heat production in the upper crust) were among the most sensitive parameters. In addition, the thermal conductivity of the Yarragadee Formation was also quite important to the value of the objective function.

We decided to estimate only those parameters that cumulatively contributed up to 95% of the total sensitivity of the objective function. We therefore were faced with estimating two parameters for the basal heat flux, the radiogenic heat production rate (HPR) rate of the upper crust, and eight thermal conductivity values. The most sensitive thermal conductivities were found in the deeper sedimentary layers, which had the most volume in the conductive model.

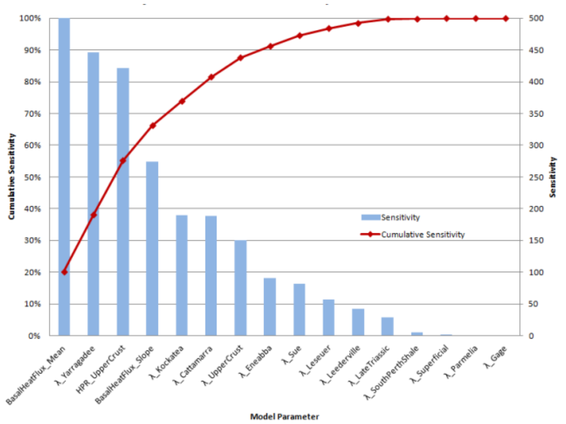

Figure 2. Sensitivity of the least-squares objective function to formation thermal conductivity [λ], radiogenic heat production [HPR] of the upper crust, and basal heat flux mean and slope.

The contribution of individual data points to simulated output is shown in Figure **3**. No evidence of bias to any of the sub-basins is shown, although the iTOUGH2 analysis did show that wells in the north sub-basin were five times as important as those in the central and south. The importance of the basal heat flux and HPR parameters are clear in this chart as well. Because there were only 15 parameters to estimate and 135 data points to provide information, sophisticated analyses such as eigenvalue grouping or singular value decomposition were not utilized in the estimation procedure.

AUTOMATIC CALIBRATION

Basal Heat Flux

Unfortunately, the parameters for the basal heat flux and the HPR of the upper crust were highly correlated to each other. It was impossible to distinguish between the two while performing automatic calibration. Therefore, we took the pragmatic approach of first estimating the basal heat flux of the combined deep and shallow models, while leaving all other parameters fixed at their prior, manual calibration values. Parameter estimation was performed in iTOUGH2 using a least squares Levenberg-Marquardt estimator. The procedure estimated a basal heat flux varying between 20 mW m^{-2} at the southern limit and 32 mW m^{-2} in the northern extent of the model. This decision allowed us to perform future calibrations with only the shallow model: the deep and shallow models are coupled only through the basal heat flux at this stage in the calibration. Forward-simulation running times were reduced by half.

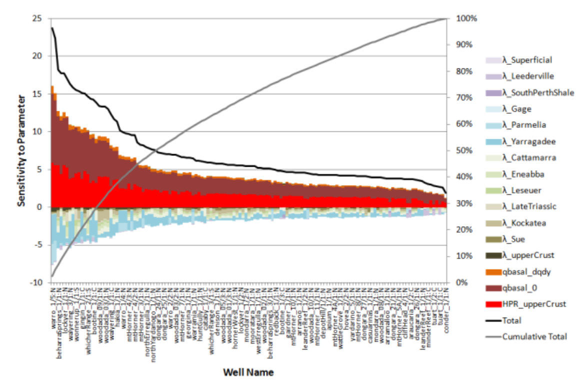

Figure 3. Sensitivity matrix plotted by wells and formation. Sub-basin is appended as a suffix to well name.

Thermal Conductivity and HPR

Least Squares Estimator

Next, we performed parameter estimations of the eight thermal conductivities and the upper crust HPR, again using a least-squares Levenberg-Marquardt estimator. To stabilize the inversion, we used the prior weighting capabilities of iTOUGH2. The manual calibration parameter was treated as a prior value. Upper and lower bounds for the parameters were determined by inspecting detailed core measurements and by comparing analogous formations worldwide (see Reid et al., 2012a, for references). Once the permissible parameter range was fixed, a standard deviation for the parameter was calculated by assuming a normal distribution and using the fixed range as ± 2 standard deviations. Note that the mean of this assumed distribution was generally not equivalent to the prior calibrated value. Moreover, directly measured thermal conductivity values were obtained with two different techniques.

iTOUGH2 calibration decreased the temperature residuals and improved the objective function by 32%. However, analysis of the temperature residuals was still disappointing. As in the manual calibration, only 55% of simulated temperatures at the wells were good. The mean residual was 0.273°C, with standard deviation of 2.8°C; an ideal model would have 0 mean and a standard deviation of 1°C. More sophisticated analysis techniques of iTOUGH2 indicated that the model failed the Fisher Model Test, or equivalently that the residual errors could not be considered to come from a stochastic distribution, and were not randomly distributed.

Least squares estimation assumes that the measurement error is the only source of error in the model system. The system error is presumed to be zero when the forward model exactly describes the physical state of the system. However, in our model, 21% of the residuals were more than 3 standard deviations away from the theoretical mean of zero, and could be considered outliers.

Physically, the conduction model assumes that heat moves in the subsurface only by a diffusive process. It does not assume the movement of heat by advectively moving groundwater, or by density-driven convection. However, there is considerable evidence to show that the aquifers of the Perth Basin do exhibit advective and convective heat transport (Sheldon et al. 2011; 2012a; 2012b). These modes of transport produce temperature profiles horizontally and in depth that are nonlinear and can have considerable deviation from the conductive profile (Rühaak et al., 2010; Sheldon et al. 2012b). Our simulator is, quite frankly, inadequate to describe the processes that produce the subsurface measurements.

Robust Andrew's Estimator

We therefore turned to a more robust estimator for calculating the model parameters (Finsterle and Najita, 1998). The Andrew's estimator discounts residuals that are far from the expected normal behaviour. As we believed that our corrected true formation temperatures had measurement error that was randomly distributed, we applied an Andrew's estimator with a parameter c=2.1. In plots below, this estimator is termed "Robust."

Again an iTOUGH2 estimation was run, but with the changes to the objective function and modifications to the Levenberg-Marquardt stepping scheme to decrease overshoot. The final estimated parameters are shown in Table **1**. After inversion, the objective function decreased by 38%, similar to the least-squares estimator but the large residual outliers are not counted in this calculation. Now, 66% of residuals are good and within 2 standard deviations of the measurement error. The overall mean residual has improved to 0.07°C, with a standard deviation of 0.66°C.

Comparison of Estimators

The residuals are plotted in histogram format in Figure **4**. Neither set of residuals appear normal; both fail the Fisher Model Test. However, the robust estimator has many more residuals within the ±2 standard deviation range.

To see whether the residuals had a trend, several analyses were performed. One example is shown in Figure **5**, where the residuals are plotted against depth. No strong depth-related trend is obvious, although a linear regression through the data shows that simulated temperatures are slightly cooler with depth, but errors are essentially uncorrelated.

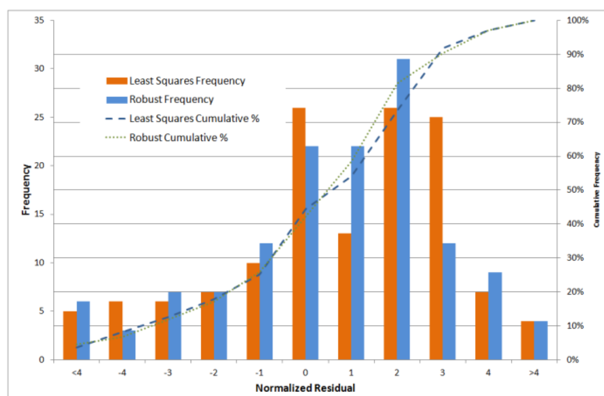

Figure 4. Histogram of temperature residuals for least squares and robust estimators.

Using the robust estimator was particularly helpful in identifying data that did not fulfill the conductive assumption, by pinpointing locations with large absolute normalized residuals. For example, Well Gingin 1 is located in the Central Perth Basin and has two high quality DST temperature measurements at -3874 m AHD and -4453 m AHD. The respective temperature measurements are 93.3 and 160°C. The local geothermal gradient between these two measurements is 115°C km^{-1}. Assuming no measurement or model error, this gradient is wildly different than the more reasonable average geothermal gradient of 25°C km^{-1} obtained from nearby Gingin 3 and reflected in other Perth Basin wells. This type of statistical analysis could be used to answer fundamental process questions such as posed by Sheldon et al. (2011).

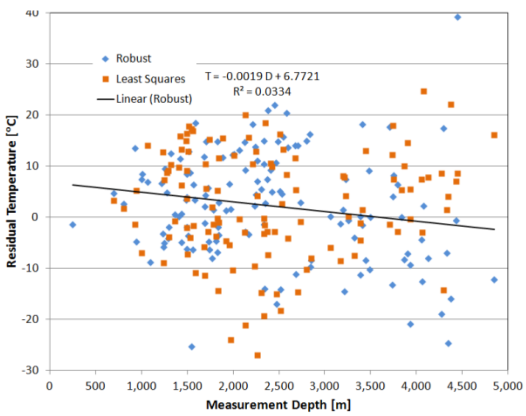

Figure 5. Scatter plot of temperature residuals versus depth.

DISCUSSION

Manual calibration of the model to available temperature data proved to be a complicated task due to the simplified rock formations and different qualities of temperature measurements. Combining the geothermal simulation performed with SHEMAT with the inverse modeling capabilities of iTOUGH2, through the recently developed PEST interface, greatly facilitated estimating model parameters.

However, the automatic estimation procedure is not a panacea for physical analysis. For example, the final results shown in Table **1** have four parameters that are restricted by the reasonable bounds applied as prior information. Additional inversions should be performed removing these bounds, to see if estimated parameters remain physically realistic. The imposed bounds are also influenced by the difference in measurement types, which can produce parameter measurements with different fundamental scales. It is difficult to reconcile these types of system error in the iTOUGH2 inversion process. Alternatively, reaching the parameter bounds in the estimation process can indicate the most fruitful areas for additional direct parameter measurements.

Another consideration raised by the inversion process is whether the highly correlated basal heat flux and radiogenic heat production from deep layers can truly be estimated from relatively shallow measurements. This ill-posed problem should be further investigated mathematically; such has been done with magnetic or seismic estimation of the Mohorovičić discontinuity, to see whether the deep parameters can be determined from near surface data.

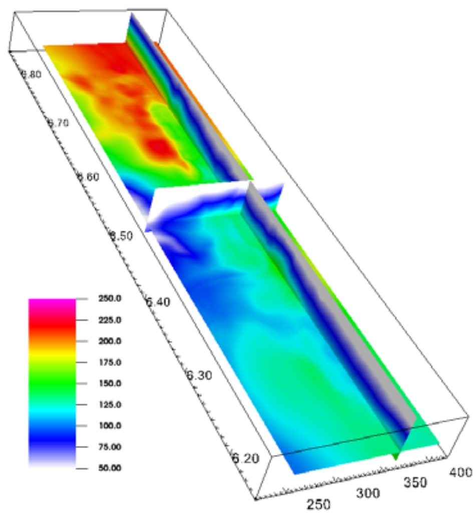

Figure 6. Simulated temperature [°C] at 5000 m depth.

The final simulated temperature field [Figure **6**] provides a picture of large-scale temperature variations in the Perth Basin, which may be used to identify possible locations of attractive geothermal resources. Extending the previously existing large-scale geothermal simulation with iTOUGH2 provided us with a more detailed insight into the sensitive parameters and data in the model, which would clearly not be possible with a simple trial-and-error calibration method. Using the gained knowledge, future work will include more detailed submodel studies on the reservoir scale including hydrogeological and geothermal processes such as advection and convection.

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